LITERATURE CITED

1. P. K. Bridson and T. P. Weirich, *J. Heterocycl. Chem.*, **25**, 1179 (1988).
2. É. I. Ivanov, A. V. Bogatskii, and K. S. Zakharov, *Dokl. Akad. Nauk SSSR*, 591 (1980).
3. T. Ohsaki, T. Kuriki, T. Ueba I. Sakakibara, and M. Asano, *Chem. Pharm. Bull.*, **34**, 3573 (1986).
4. L. P. Kulev and R. N. Gireva, *Zh. Prikl. Khim.*, **30**, 811 (1957).
5. E. Godefroi, C. Eyeken, and C. Westering, *J. Org. Chem.*, **29**, 3707 (1964).

FORMATION OF DERIVATIVES OF 1,2,4-TRIAZOLOQUINAZOLINES IN THE REACTIONS OF 3-AMINO-1,2,4-TRIAZOLES WITH CYCLOHEXANONE

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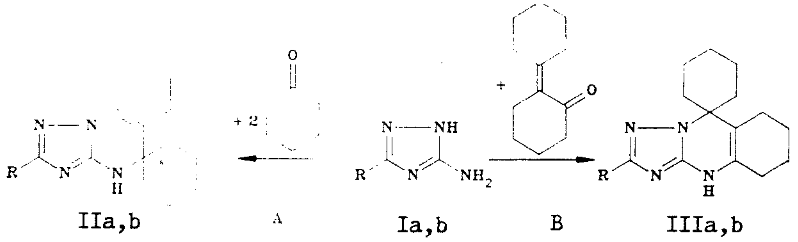
It is known [1, 2] that the reactions of binucleophiles with ketones containing the activated methyl or methylene group, or with the products of the self-condensation of these ketones, may lead to one and the same substance. We established that the boiling of the solutions of the 3-amino-1,2,4-triazoles (Ia, b) and cyclohexanone in DMF in the course of 4-6 h (reaction A) leads to the formation of the compounds (IIa, b), for which the mass spectra and the data of the elemental analysis indicate that the condensation of the ketone with the amine takes place with the 2:1 molar ratio, and with the cleavage of 2 moles of water.

Under the analogous conditions, the condensation of the amines (Ia, b) with 2-cyclohexylidenecyclohexane (reaction B) leads to the formation of the substances (IIIa, b) having the same composition and molecular mass as the compounds (II). However, according to the data of the TLC, the IR spectra (the region of the fingerprints), and the PMR spectra, the compounds (II) and (III) are different discrete substances; this permitted the proposition that the isomeric derivatives of 1,2,4-triazoloquinazolines are formed in the reactions A and B.



I–III a R=H, b R=NH$_2$

The choice between the structures (II) and (III) for the substances obtained was made on the basis of the direction of the cyclocondensation of 3-amino-1,2,4-triazole with α,β-unsaturated ketones (corresponding to the reaction B), which we established previously [3], as well as by the comparison of the position of the signal of the imine proton in the PMR spectra of these compounds. In the case of the substances (IIIa, b), the values of δ_{NH} are typical of the derivatives of 4,7-dihydro-1,2,4-triazolo[1,5-*a*]pyrimidine [3], whereas the signal of the imine proton is noticeably displaced to the region of higher field in the spectra of the compounds (IIa, b). These facts indicate the varying disposition of the imino group in relation to the C=C bond in the compounds under comparison: The enamine character of this group in the compounds (IIIa, b) determines its high acidity and, consequently, also the higher values of the δ_{NH}.

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TABLE 1. Characteristics of the Compounds (IIa, b) and (IIIa, b)

Compound	mp, °C	UV spectrum		IR spectrum, ν C=C, cm^{-1}	PMR spectrum, δ, ppm				Yield, %
		λ_{max}, nm	$\varepsilon \cdot 10^{-3}$		1H, s, CH	1H, s, NH	2H, s, NH_2	18H, m $(CH_2)_n$	
IIa	218	258	3,4	1675	7,89	7,05	—	1,1 . . . 2,2	54
IIb	197 . . . 198	268	5,4	1680	—	6,85	4,85	1,1 . . . 2,3	57
IIIa	233 . . . 234	255	3,7	1682	7,76	9,90	—	1,0 . . . 2,1	56
IIIb	251	263	3,3	1682	—	9,95	4,90	1,1 . . . 2,2	61

The difference in the direction of reactions A and B clearly shows that the self-condensation of two molecules of cyclohexanone cannot be the first stage of its reaction with the amines (Ia, b).

LITERATURE CITED

1. A. R. Butler, J. Hussain, and E. Leitch, *J. Chem. Soc., Perkin 2*, No. 1, 106 (1980).
2. V. D. Orlov and S. M. Desenko, *Khim. Geterotsikl. Soedin.*, No. 12, 1673 (1985).
3. V. D. Orlov, S. M. Desenko, K. A. Potekhin, and Yu. T. Struchkov, *Khim. Geterotsikl. Soedin.*, No. 2, 229 (1988).

ADDITION OF 4-NITROBENZONITRILE-N-OXIDE TO DERIVATIVES OF α-METHYLENELACTONES

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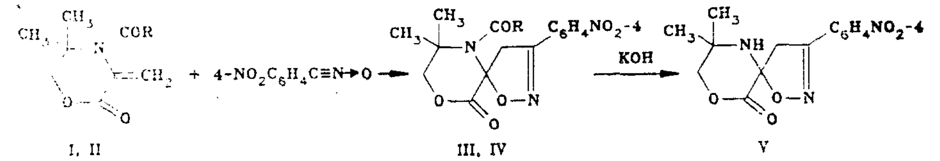
The N-acylated α-methylenelactones (I) and (II) readily participate in the reaction of the cycloaddition with 4-nitrobenzonitrile-N-oxide resulting in the formation of the spirocyclic derivatives (III) and (IV). The reaction proceeds at room temperature in acetonitrile:



I, III $R=C_6H_5$; II, IV $R=C_6H_5CH_2O$

The addition proceeds regiospecifically and only leads to the isomer in which the oxygen atom of the isoxazoline ring is connected to the spiro atom. The orientation of the addition is confirmed by the data of the PMR spectra, in which the signals of the methylene protons of the isoxazoline ring appear in the region of 4 ppm; this is characteristic of the methylene group at the position 4 [1].

The amide (III) is readily deacylated by the action of aqueous alkali; the spirocyclic system is thereby retained.

4-Benzoyl-5,5-dimethyl-4'-(4-nitrophenyl)-2-oxomorpholine-3-spiro-5'-(2-isoxazoline) (III). mp 209-211°C (from CH_3CN). PMR spectrum (DMSO-D_6): 1.27 and 1.46 ppm (3H each, s, CH_3), 3.62 and 4.29 ppm (1H each, d, J = 19 Hz, CH_2), 4.33 and 4.62 ppm (1H each, d, J = 12 Hz, CH_2), 7.1-7.5 ppm (5H, m, C_6H_5), and 7.62 and 8.16 ppm (2H each, d, J = 9 Hz, C_6H_4).

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